Federal Government Prospective on High End Computing

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The Future of High Performance Computing:
Leadership and Technological Advancement
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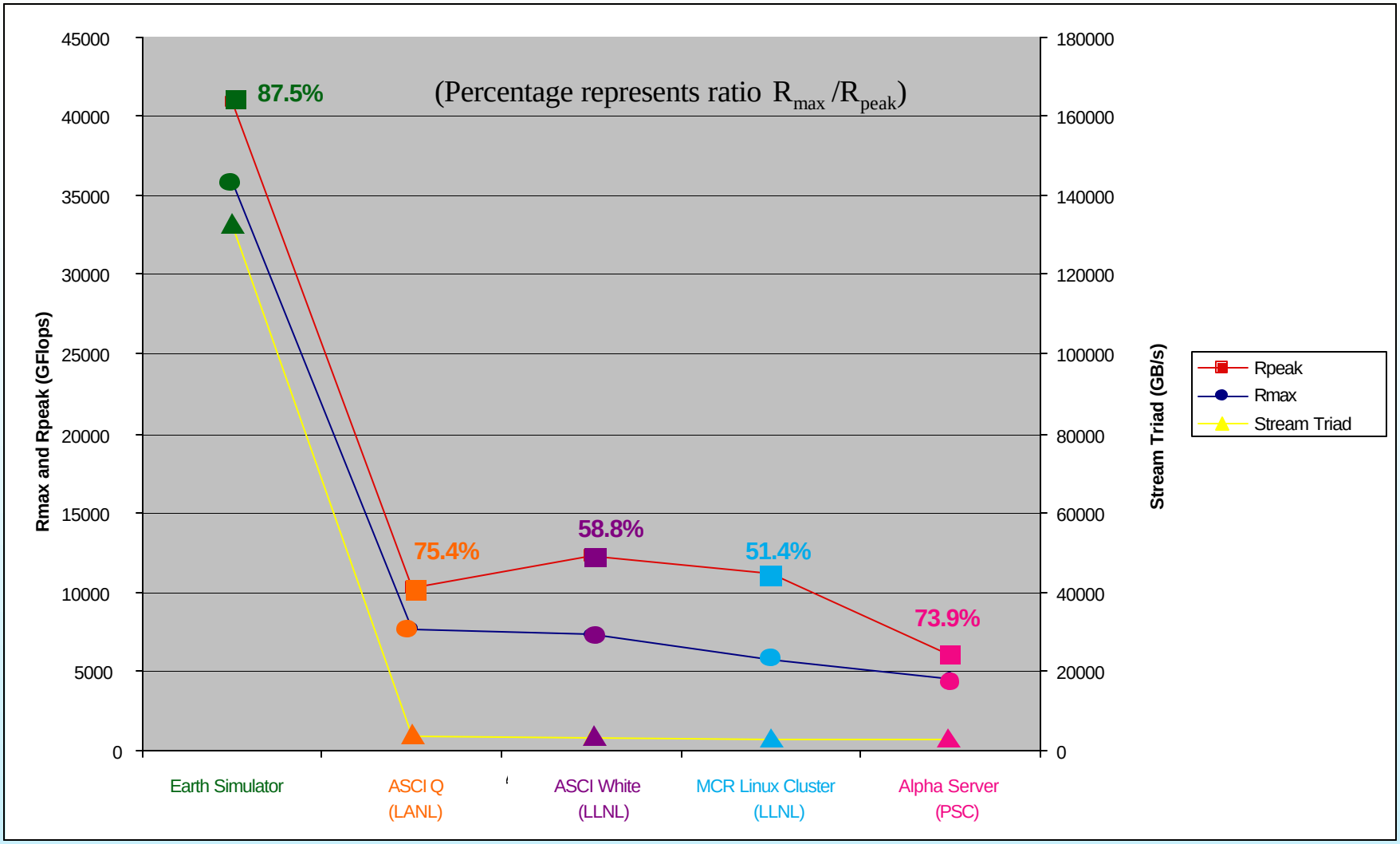
Networking and Information Technology Research and Development (NITRD) Program

- Coordinated, focused long-term interagency R&D in information technologies
- Evolved from the Federal HPCC, CIC, NGI, and IT R&D programs
- $2 billion multi-agency NITRD Program
  - 12 agencies and departments coordinated via a “virtual agency” coordination/management structure
    - AHRQ, DARPA, DOE/NNSA, DOE/SC, EPA, NASA, NIH, NIST, NOAA, NSA, NSF, ODDR&E
  - Coordinated by the National Coordination Office for Information Technology Research and Development
- Assessed by the President’s Information Technology Advisory Committee

Performance Measures of Selected Top Computers



R_{peak} and R_{max} data from Top500.org Stream Trend data from IDC

Several Federal Agencies Have Recently Examined High End Computing Needs (1)

- Agencies include:

  DARPA, DOE/NNSA, DOE/SC, EPA, NASA, NIH, NIST, NOAA, NSA, NSF, ODDR&E
- They are mostly using COTS-based HEC*
- Most expect COTS-based HEC to be acceptable in near term, however:
  - Time-to-solution becoming too long
    - Too hard to program; too hard to optimize
  - For many problems, computing efficiency is dropping as number of processors increases
    - Affects cost-to-solution, time-to-solution
  - Memory performance (latency/bandwidth/size) is often the limiting factor
  - For some applications I/O system performance is limiting
- Examples of HEC application areas with Federal interest
  - Nuclear stockpile stewardship (multi-discipline physics models)
  - Global and regional climate modeling and weather forecasting
  - Ocean state prediction
  - Geophysics (earthquakes, volcanoes, landslides, plate tectonics, magneto-dynamics)
  - Astrophysics (star and galaxy dynamics)
  - Aeronautics (propulsion, air-frames, re-entry vehicles)

*Note: In this talk COTS-based HEC refers to systems based on COTS technology, e.g. derived from workstations or SMPs. Custom systems can also be built with COTS components. These are not considered COTS-based in this context.

Several Federal Agencies Have Recently Examined High End Computing Needs (2)

- Examples (continued)
  - Engineering design of ships, land vehicles, buildings
  - Weapon designs and weapon effects
  - Armor design
  - Survivablility/stealthiness design
  - Signal and imagining processing
  - Cryptanalysis
  - Molecular modeling for chemical risk assessment
  - Biophysics (e.g., protein folding)
  - Pharmacology
  - Quantum chemistry
  - Materials modeling and design (e.g., concrete)
  - Quantum chromodynamics
- Some important applications/algorithms are not amenable to COTS-based HEC
  - Primarily due to non-local memory reference (e.g., long vectors requiring gather-scatter operations)

Examples of Applications for Which COTS-Based HEC May be Unsuitable

- Hypersonic air-breathing propulsion
  - Needs high memory-to-CPU bandwidth for multi-disciplinary analysis
- Reusable launch vehicle design
  - Needs high memory-to-CPU bandwidth
- Protein folding
  - Poorly parallelizable
- Cryptoanalysis
  - Needs fast flat-memory model
- Climate data assimilation
  - Part of problem not easily parallelizable, needs high memory-to-CPU bandwidth

Agency Conclusions

- Further progress in HEC will require balanced, coordinated effort in:
  - Research, development, and engineering of new HEC architectures and systems
  - Procurement of new COTS-based and custom systems
  - Better software (systems, middleware, and applications)
  - Better domain science (mathematics and algorithms)
- HEC is a decreasing part of the technical computing marketplace.
- COTS-based HEC is largely based on technologies developed for low- and mid-range markets (SMP nodes, low bandwidth interconnects).
- Market pressure may result in future COTS-based systems being less responsive to HEC needs.
- Federal funding of highest-performing HEC, including development of new systems, may be required.

High End Computing (HEC) in President's FY 2004 Budget

"Due to its impact on a wide range of federal agency missions ranging from national security and defense to basic science, high end computing—or supercomputing—capability is becoming increasingly critical. Through the course of 2003, agencies involved in developing or using high end computing will be engaged in planning activities to guide future investments in this area, coordinated through the NSTC. The activities will include the development of interagency R&D roadmap for high-end computing core technologies, a federal high-end computing capacity and accessibility improvement plan, and a discussion of issues (along with recommendations where applicable) relating to federal procurement of high-end computing systems. The knowledge gained for this process will be used to guide future investments in this area. Research and software to support high end computing will provide a foundation for future federal R&D by improving the effectiveness of core technologies on which next-generation high-end computing systems will rely."

High End Computing Revitalization Task Force (HECRTF) Charge

- Rationale: High End Computing (HEC) increasingly critical
- HECRTF coordinated through National Science and Technology Council (NSTC)
- To develop a five-year plan that can guide future Federal HEC investments
- Plan will lay out an overall strategy for these investments
- Seek wide participation by Federal agencies developing or using HEC
- Final report to be completed by August 2003, in time to serve as input to FY 2005 budget
- May 1: Rough draft
- June 1: Draft
- August: Final report
- Outreach strategy being developed

HECRTF Organization

- Task Force - Oversight and guidance
- Task Groups - Specific issue
  - Integration
  - Core Technologies Research & Development
  - Capacity, Capability, and Accessibility
  - Procurement of Federal HEC Systems
- Coordination and support from NCO

For Further Information

Please contact us at:

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Or visit us on the Web:

www.itrd.gov

Back Up

National Coordination Office (NCO) for Information Technology Research and Development (IT R&D)

Mission: To formulate and promote Federal information technology research and development to meet national goals

- NCO Director reports to the Director of the White House Office of Science Technology Policy (OSTP)
- Coordinates planning, budget, and assessment activities for the Federal multiagency Networking and Information Technology Research and Development (NITRD) Program
- Supports the six technical Coordinating Groups (CGs) that report to the Interagency Working Group (IWG) on IT R&D
  - Research planning workshops, conferences, and meetings
  - Presentations, white papers, and research reports
- Provides technical and administrative support to the IWG and to the President's Information Technology Advisory Committee (PITAC)
- Informs the public of Federal achievements and challenges in IT R&D
  - Maintains a Web site
  - Publishes annual budget documents in cooperation with the IT R&D agencies
  - Publishes PITAC reports